Multidisciplinary Approaches to Science for Nanoscale Interfaces

A Report on the NECIS Workshop held on September 6-8, 2006 at Bishop's Lodge Ranch, Santa Fe, New Mexico

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Abstract

This report summarizes the technical work presented, and issues discussed, at a workshop held at the Bishop's Lodge Ranch in Santa Fe, New Mexico from September 6 to 8, 2006. This workshop was sponsored by the newly formed Nanoscience, Engineering, and Computation Institute at Sandia (NECIS). NECIS' primary mission is to support Sandia National Laboratories' response to the American Competitiveness Initiative (ACI) by facilitating research and the rapid transfer, application, and integration of new knowledge between the nanoscience, nanoengineering, and high-performance modeling and simulation fields that are critical to Sandia's national security mission. This workshop's goal was to provide a forum for selected scientists and engineers from the nation's top universities and research laboratories to discuss pressing issues on interfaces in nanoscience and technologies. The goal of this workshop was to identify, define and debate the key issues regarding materials interfaces that are limiting progress in the development of nanotechnology. Discussion centered on increasing awareness of experimental, theoretical and computational approaches towards understanding the science of nanoscale interfaces.

Information on this workshop can be found at the website:
http://www.cs.sandia.gov/CSRI/Workshops/2006/NECISWorkshop/

Keywords: interfacial science; nanoscience; nanoengineering; innovation .

Introduction

In the Spring of 2006, researchers at Sandia National Laboratories established the Nanoscience, Engineering, and Computation Institute at Sandia (NECIS) in order to jumpstart a new initiative in nanotechnology designed to cross-fertilize and integrate nanoscale physical and biological sciences with computational science to inspire and expedite breakthroughs in nanotechnology. Computational science, which encompasses both computer science and mathematics, is a fundamental capability that will enhance innovation in the emerging field of nanoengineering. However, application of computational science in this nascent field requires new approaches to research training to tackle fundamental challenges in nanosystems modeling and simulation that is coordinated with leading-edge, innovative experiments for efficient development and validation of disruptive nanotechnologies. NECIS was formed to address these challenges and to support Sandia National Laboratories' response to the American Competitiveness Initiative (ACI) by facilitating research and the rapid transfer, application, and integration of new knowledge between the nanoscience, nanoengineering, and high-performance modeling and simulation fields that are critical to Sandia's national security mission.

Among the many activities undertaken by NECIS' leadership are technical workshops to educate laboratory staff, academic faculty, and industry researchers in novel approaches to nanoengineering and to facilitate new collaborations between these sectors in order to initiate innovative research efforts. Between September 6 and 8, 2006, the first of these workshops was conducted on the topic of **Multidisciplinary Approaches to Science for Nanoscale Interfaces**. The workshop was organized by Jonathan Zimmerman, Steve Plimpton, Neville Moody, Rich Lehoucq, Jean Lee, Eliot Fang, and Scott Collis, thereby representing a mixture of Sandia leadership (Lee, Fang, Collis) and technical staff (Zimmerman, Plimpton, Moody, Lehoucq) with expertise in both experimental and computational methods. This workshop's goal was to provide a forum for selected scientists and engineers from the nation's top universities and research laboratories to discuss pressing issues on interfaces in nanoscience and technologies. The objectives for this collaborative event were to establish a common knowledge foundation for this critical area of research, explore how the practices of verification and validation function in scientific development, and identify paths of collaboration and innovation for this community to create a tapestry of methods in experimentation, computation and modeling and simulation.

In order to identify, define and debate the key issues regarding materials interfaces that are limiting progress in the development of nanotechnology, abstracts were solicited from the pool of invited participants to address, if not answer, the following questions:

1. What are the state of the art tools and techniques to understand interfacial structure and phenomena?
2. What are the major challenges of these methods that prevent the scientific community from doing predictive science?
3. Can we identify the means to gauge the importance of the phenomena we study and the validity of the methods we use?
4. What are some new ways in which researchers with varied expertise, techniques and working environments can collaborate to stimulate innovative research?
5. How do we prepare both ourselves, and the next generation of scientists to do innovative research in interfaces?

A total of seven, one-hour presentations, and the subsequent discussions centered on increasing awareness on experimental, theoretical and computational approaches towards understanding the science of nanoscale interfaces.

Workshop Program

Wednesday, September 6th

4:00 - 6:00 pm: Hotel check-in

6:00 - 6:30 pm: Workshop registration and poster viewing

6:30 - 7:30 pm: Dinner and poster viewing

Session 1: 7:30 - 9:00 pm

7:30 - 7:40 pm: Welcome and opening remarks by Jon Zimmerman

7:40 - 8:20 pm: Technical Speaker #1: Bruce Bunker, Sandia National Laboratories, *Interfacial Issues in Integrated Nanotechnologies*

8:20 - 9:00 pm: Discussion on expectations for workshop

Thursday, September 7th

7:30 - 8:30 am: Breakfast and workshop registration

Session 2: 9:00 am - 12:00 pm

9:00 - 9:40 am: Technical Speaker #2: Ken Liechti, University of Texas at Austin, *Experimental and Computation Issues Related to Adhesion, Friction and Wear of Surfaces Modified by Self-Assembled Monolayers*

9:40 - 10:10 am: Discussion

10:10 - 10:30 am: Coffee break

10:30 - 11:10 am: Technical Speaker #3: Wing Kam Liu, Northwestern University, *Challenges and Limitations in Multiscale Predictive Scientific Simulations*

11:10 - 11:40 am: Discussion

12:00 - 1:30 pm: Lunch, poster viewing and free time

Session 3: 1:30 - 4:10 pm

1:30 - 2:10 pm: Technical Speaker #4: Qiang Du, Pennsylvania State University, *Recent Progress on the Phase Field Modeling of Interfacial Problems*

2:10 - 2:40 pm: Discussion

2:40 - 3:00 pm: Coffee break

3:00 - 3:40 pm: Technical Speaker #5: Alec Talin, Sandia National Laboratories, *Role of Surfaces in Nanowire Electronics, Photonics and Sensors: Challenges and Opportunities*

3:40 - 4:10 pm: Discussion

4:10 - 6:00 pm: Free time

6:00 - 7:00 pm: Dinner and poster viewing

Session 4: 7:00 - 8:10 pm

7:00 - 7:40 pm: Technical Speaker #6: Hanchen Huang, Rensselaer Polytechnic Institute, *Synergy of Atomistic Simulations and Experiments vs. Multiscale Modeling*

7:40 - 8:10 pm: Discussion

Friday, September 8th

7:30 - 8:30 am: Breakfast

Session 5: 9:00 am - 12:00 pm

9:00 - 9:40 am: Technical Speaker #7: Stephen Foiles, Sandia National Laboratories, *Atomistic Simulation of Interfaces: Does the Emporer have any Clothes?*

9:40 - 10:10 am: Discussion

10:10 - 10:30 am: Coffee break

10:30 am - 12:00 pm: Expanded discussion targeted on workshop questions 4 and 5

12:00 - 1:15 pm: Lunch

Session 6: 1:30 - 3:00 pm

1:30 - 3:00 pm: Discussion and dialogue on ideas for workshop follow-up

Workshop Participants

Name, Affiliation

Mark Alper, Lawrence Berkeley National Laboratory

Helgi Adalsteinsson, Sandia National Laboratories - CA

David Bahr, Washington State University

Pavel Bochev, Sandia National Laboratories - NM

Bruce Bunker, Sandia National Laboratories - NM

Scott Collis, Sandia National Laboratories - NM

Eilene Cross, Sandia National Laboratories - CA

Paul Crozier, Sandia National Laboratories - NM

Qiang Du, Pennsylvania State University

Don Estep, Colorado State University

H. Eliot Fang, Sandia National Laboratories - NM

Jacob Fish, Rensselaer Polytechnic Institute

Stephen Foiles, Sandia National Laboratories - NM

Max Gunzburger, Florida State University

Hanchen Huang, Rensselaer Polytechnic Institute

Jean Lee, Sandia National Laboratories - CA

Richard Lehoucq, Sandia National Laboratories - NM

Kenneth Liechti, University of Texas at Austin

Wing Kam Liu, Northwestern University

Neville Moody, Sandia National Laboratories - CA

Xiaobo Nie, Johns Hopkins University

Michael Parks, Sandia National Laboratories - NM

Steven Plimpton, Sandia National Laboratories - NM

Christopher San Marchi, Sandia National Laboratories - CA

Mark Shephard, Rensselaer Polytechnic Institute

Ralph Smith, North Carolina State University

Mark Stevens, Sandia National Laboratories - NM

Alec Talin, Sandia National Laboratories - CA

Stephen Thomas, Sandia National Laboratories - NM

Willliam Tong, Hewlett-Packard

Greg Wagner, Sandia National Laboratories - CA

Edmund Webb III, Sandia National Laboratories - NM

Xiaowang Zhou, Sandia National Laboratories - CA

Jonathan Zimmerman, Sandia National Laboratories - CA

Technical Presentations

Bruce Bunker, Sandia National Laboratories

Interfacial Issues in Integrated Nanotechnologies

The lead speaker for the workshop was Bruce Bunker, a Sandia technical staff member who has been heavily involved in the Center for Integrated Nanotechnologies (CINT). His talk discussed some of the activities related to nanoscale interfaces that CINT supports; in particular, his current involvement in CINT is focused on their thrust areas of Complex Functional Materials and Nano-Bio Interfaces. Bruce provided several examples of research efforts that have the goal of understanding how water, salts, and other elements inherent to the environment modify the interfacial behavior of nanomaterials. He also explained what experimental methods are used to perform this research, *e.g.* Atomic Force Microscopy (AFM) and Interfacial Force Microscopy (IFM), and displayed the conceptual and numerical models that are being developed to explain mechanisms operational in these systems.

During his talk, Bruce listed many of the challenges that face research conducted by CINT scientists, including:

- Quantifying to what extent can such complex assembly and functionality be achieved in man-made nanomaterials?
- How do environmental elements like water order near nano-scale interfaces and surfaces, and how does that ordering influence transport and other processes?
- To what extent can models be believed? Also, have we even successfully identified what tools are needed to interrogate these systems?

The subsequent discussion attempted to answer the final challenge by suggesting that an iterative coupling of experiment and modeling & simulation is essential towards gauging the validity of research conducted. It was also proposed that, in this manner, theoretical developments should guide the path followed by experimentation rather than simply being used to study what has already been done in experiments and to use them for validation.

Part of the discussion that followed Bruce's talk was used to clarify the expectations of the workshop participants, particularly those from the academic community. Among the issues raised was:

- The desire for more information on how Sandia goes about conducting multidisciplinary research.
- Whether inter-disciplinary training was advantageous with regard to training the next generation of scientists as compared with multidisciplinary partnerships?
- Is there a way to change the perspective of funding agencies and research calls from short-term projects to longer-term collaborations?
- How do we generate excitement and instill passion in our youth with regard to scientific and engineering research and development?

Ken Liechti, University of Texas at Austin

Experimental and Computation Issues Related to Adhesion, Friction and Wear of Surfaces Modified by Self-Assembled Monolayers

Ken Liechti provided the workshop group with a focused presentation on the work that he, his collaborators, and others have done on using Self-Assembled Monolayers (SAMs) to increase the effective fracture toughness of nanoscale interfaces over the intrinsic toughness of these materials by a factor of 4-5. His talk covered both the experimental methods used to examine interfaces such as epoxy/sapphire, and some attempts to develop traction-separation laws for use in cohesive surface zone (CSZ) models and finite element analysis. He noted that while such laws realistically depend on mode-mixity, *i.e.* the relative amount of shear versus normal displacement that the interface is being subjected to, models to capture this dependency are still lacking and that simpler models are only sufficient in limited cases.

During his talk, Ken identified some critical issues that need to be resolved with regard to research in this field. These include:

- **SAM deposition**
  This includes the areas of processing of SAMs, the performance of diagnostics, and

modeling of the deposition process. Processing included both hydrous and anhydrous methods and details surrounding the surface preparation and post-processing were also discussed. Methods for SAM diagnostics include X-ray Photoelectron Spectroscopy (XPS), Ellipsometry, AFM, IFM and Scanning Tunnel Microscopy (STM). While these methods all have value, Ken expressed a need for improved methods that can positively identify when and where a SAM has formed. Ken assured the participants that mechanical indentation testing of SAM-coated interfaces at multiple locations, via IFM, is used to sufficiently guarantee that the coating is uniform and possesses a minimum of defects. Regarding modeling of the deposition process, Ken discussed some recent research using the phase field approach to predict patterns of the deposited molecules. Such an approach is used to help overcome the time-scale issues inherent to more fundamental modeling methods like empirical potential atomistic simulations.

- **SAM probing**
  Ken discussed in more detail the tools and techniques used for normal, shear and combined normal-shear loading in quantifying the mechanical properties of these materials. Particular attention was given to the Interfacial Force Microscope, developed by Jack Houston and colleagues at Sandia.

- **Analysis of SAMs**
  Ken reviewed both atomistic and continuum approaches towards understanding the constitutive behavior of SAM films and the resulting deformation properties. Continuum approaches included by analytical solutions from contact mechanics, and numerical solutions using finite element analysis. Ken particularly noted how non-linear constitutive relationships, such as hyperelastic and hypoelastic material models, are essential towards accurately representing the deformation of these systems and that linear-elastic models are entirely insufficient.

Ken concluded his talk by discussing outstanding issues such as patterning binary SAMs and including the effects of defects in SAM processing, the need for advanced, high-speed techniques in SAM probing, and the next stage of model development to include effects such as phase separation, water and the ability to simulate the correct time scales for sliding and the correct length scales for wear.

Wing Kam Liu, Northwestern University

Challenges and Limitations in Multiscale Predictive Scientific Simulations

Wing Kam Liu presented an in-depth look at some materials interface problems that present unique challenges for theorists and modelers with expertise in multiscale simulation methods:

- **Radiation Effects on MEMS**
  Wing Kam noted how verified and validated predictive methodologies are vitally needed to qualify and quantify how radiation accelerates the diffusion of materials leading to aging effects, material instabilities, and microstructure evolution in nano- and microscale systems, *i.e.* the interaction of charged particles with crystalline microstructures. Wing Kam outlined the simulation methods that must be combined in order to develop a fully predictive simulation code, including first-principle calculations, molecular dynamics (MD), Monte Carlo (MC), combined MD-MC, phase field models, and methods that incorporate statistics for a dynamic continuum.

- **Materials Instability, Aging and Microstructure Evolution**
  The topic includes combinations of thermal-electrical-mechanical properties that can lead to material instabilities and degradation of material microstructure. Wing Kam proposed that multiscale methods are necessary to model phenomena such as thermal cycling, dynamic loading, adhesion, stiction, electrical arcing, void formation and movement, and grain boundary evolution. He noted in particular several barriers to constructing accurate models including the seamless coupling of MD to MC, incorporating the effect of dislocations and grain boundaries on diffusion within solids, reliable methods to provide input parameters for MC and lattice-Kinetic Monte Carlo (LKMC) methods, and the implementation of advanced multiscale methods within reliable material simulation codes.

- **Novel Materials Design**
  For this portion of his talk, Wing Kam demonstrated the use of multiscale simulation methods to aid the design of material interfaces. He presented one example in which the accurate representation of microvoids is an essential ingredient towards modeling shear localization near a material interface, and another example for which the effect of microstructure on fracture toughness is qualified and quantified.

- **Integrated Software Design**
  Wing Kam noted that not only is the construction of accurate models to represent physical phenomenon extremely challenging, but equally demanding is the task of implementing the wide variety of modeling methods that operate at various length and

time scales into a single, integrated software product. Wing Kam presented a comprehensive list of quantum, atomistic, phase field and finite element simulation codes in addition to codes that couple these methods and others that perform uncertainty quantification. Wing Kam pointed out the barriers to this integration process such as scalability for parallel computing and difficulty encountered when combining different computational tools.

Wing Kam also briefly discussed the importance of, and barriers to, verification, validation and uncertainty quantification. In particular, he mentioned that work is still underway with regard to determining how such concepts should be applied to multiscale modeling techniques. For example, an outstanding task is the application of stochastic methods on scale-bridging formulations, *e.g.* coupled atomistic-continuum simulation approaches.

Qiang Du, Pennsylvania State University

Recent Progress on the Phase Field Modeling of Interfacial Problems

The next speaker, Qiang Du, provided the workshop group with a detailed perspective on a specific modeling approach, phase field modeling, how it is applied to the specific case study of vesicle membranes, and what are some challenges towards using it as a predictive simulation tool. He showed the underlying formulation that combines the generic phase field approach with a bending elasticity model, and how the resulting method can be effectively applied to simulate single and multi-component vesicles in biological systems. Qiang also discussed how this method can be applied to fluid systems in nano- and microscale systems. Of particular relevance to the workshop was the issue raised of constructing and implementing efficient numerical algorithms. Qiang reviewed numerical analysis methods such as finite difference, finite element and spectral methods, and emphasized the need for improvement on these methods and for improved schemes for retrieving topological information within a general diffuse-interface framework.

Alec Talin, Sandia National Laboratories

Role of Surfaces in Nanowire Electronics, Photonics and Sensors: Challenges and Opportunities

Alec Talin returned the workshop's attention to experimental methods for studying nanoscale surfaces and interfaces by presenting an interesting talk on the fabrication, analysis and modeling of both III-V semiconductor and silicon nanowires. During his talk, Alec specifically noted how surfaces have a significant impact on the electrical performance of the nanowires, and since nanowires possess very large surface-to-volume ratios, attention to this detail is critical. For example, surface bonding states have the effect of 'pinning' the Fermi level thereby causing depletion of charge carriers. For GaN nanowires, this depletion leads to unique characteristics making them promising for use in UV photodetectors. Alec also discussed how other unique attributes of nanowires, such as sensitivity of electrical and optical properties to the environment make them ideal for use in chemical and biological agent sensors. Alec also mentioned the difficulties regarding using nanowires in applications, such as the lack of a practical, robust and reproducible method for integrating nanowires into MEMS circuitry.

With regard to modeling, Alec presented analytical and numerical models currently used to reproduce charge transfer properties of nanowires. However, Alec also noted a specific example involving Si nanowires in a chemical sensor for which modeling did not accurately predict the improvement in performance achieved by changes in geometry of the sensor material components. This was a perfect example in which the value of improved modeling capability would be of tremendous benefit to not only understand a physical system, but direct what information experiments should be targeted to obtain.

Towards the end of his talk, Alec presented a list of challenges and opportunities with regard to nanowires including:

- Obtaining detailed quantification, both experimentally and with models, of surface structure and reconstruction.

- Conducting more detailed studies on surface states, nanowire structure after passivation, and core-shell structures.

- Qualifying and quantifying the effect of adsorbates on nanowire surfaces.

Hanchen Huang, Rensselaer Polytechnic Institute

Synergy of Atomistic Simulations and Experiments vs. Multi-scale Modeling

Following the second group dinner of the workshop, Hanchen Huang provided an enriching and entertaining talk discussing the synergy that exists between experiments on, and atomistic simulations of, nanoscale interfaces. He emphasized that this synergy exists by attempting to combine three pieces of fundamental physics: surface kinetics, geometrical shadowing, and stacking fault (and twin) formation. Specifically, he combined these pieces to enable atomistic simulation methods to model the self-assembly of nanorods, showing how these ingredients are essential towards quantitative agreement with experimental studies of nanorod formation.

Hanchen also provided a second example of this synergy, that of Cu thin films. This example was not presenting another case of model validation, but rather was used to identify the various length and time scales that require valid material models. For instance, while atom-by-atom deposition and the formation of nanoislands might be captured with existing atomistic simulation techniques (processes taking on the order of nanoseconds), the full formation of planar films with nano- and microscopic grains are at much larger time scales inaccessible to molecular dynamics. Such simulations required more robust techniques such as lattice kinetic Monte Carlo.

To conclude, Hanchen pointed out the evolution in the scientific community's expectation of the value associated with modeling and simulation. Whereas at one point it was believed that modeling and simulation would be capable of one day replacing experiments, the current viewpoint is more moderate by anticipating that such methods can reveal mechanisms, thereby augmenting experimental studies, as well as to design and discover new material combinations and structures.

Stephen Foiles, Sandia National Laboratories

Atomistic Simulation of Interfaces: Does the Emperor have any Clothes?

The final technical presentation for the workshop was given by Stephen Foiles. Stephen described several specific examples of how atomistic simulation methods have been applied to understand the fundamental physics of nanoscale interfaces, as well as the limitations of these methods and the challenges that need to be overcome to create predictive nanoengineering models:

- Modeling the structure of a Ag(111) thin film on a Ru(0001) substrate required not only accurate inter-atomic potentials, but insight drawn from both physical intuition and experiment. Stephen raised the question as to whether calculations would ever be able to accurately predict the interfacial structure in the absence of corresponding experiments.

- Using combinations of high resolution transmission electron microscopy (HRTEM) and atomistic simulations to discover structural details of specific grain boundaries in FCC metals. Once again, Stephen pointed out that synergistic application of simulation and experiment was needed to full understand these structures.

- Several cases demonstrating the segregation and energetics of impurities near grain boundaries in polycrystalline materials. Stephen showed that while empirical inter-atomic potentials such as the Embedded Atom Method (EAM) enable the calculation of 'large-scale' systems, they sometimes fall short in predicting accurate energies. In contrast, more fundamental methods such as density functional theory (DFT) are limited with regard to both the system size they can be used on in a computationally efficient manner, and with regard to their direct application of statistical methods.

- Understanding the factors that influence grain boundary mobility, noting how a mesoscale paradigm was necessary to account for the dependence of mobility on grain boundary misorientation angle.

Stephen then went on to discuss the many outstanding challenges that remain for the atomistic simulation of interfaces such as how to handle combinations of continuous and discrete variables that are used to describe interface structure, that the dynamic properties and thermodynamics have only begun to be explored, and that nanoscale systems inherently contain confining geometries which may alter the behavior of material models from that seen for planar interfaces.

Stephen concluded his talk by leading the workshop group through a discussion on what expectations do researchers have with regard to needing atomistic simulations to be predictive. In particular, we noted that, as a community, we need to do a better job of acknowledging where we are in the spectrum between basic understanding and predictive capability, and more activities aimed at identifying what is needed for consistency as larger-scale models are used.

Discussion on Motivating Questions

The workshop discussions held on late Friday morning and early Friday afternoon focused on distilling the information communicated during the technical presentations into answers for our workshop's motivating questions.

What are the state of the art tools and techniques to understand interfacial structure and phenomena?

The workshop participants collectively revisited the technical presentations and identified the tools and techniques mentioned:

- Bruce Bunker: AFM imaging probes, Interfacial Force Microsocpy, surface interaction models (Van der Waals), reflectometry of water and salts near nylon surfaces, integrated sensors, discovery platforms.
- Ken Liechti: Crack opening interferometry, Cohesive Zone Surfaces and Finite Element analysis, friction test apparatus, MD of SAMs materials, diagnostic techniques including XPS, AFM, IFM, STM, hypoelastic material models.
- Wing Kam Liu: MD, MC, combined MD-MC, LKMC, continuum mechanics / FEA: IEFEM, XFEM, phase field models, TB-LMTO, FLAPW (DFT), UQ methods.
- Qiang Du: Phase field models, level-set methods, efficient numerical algorithms: FD, FE, spectral methods.
- Alec Talin: CVD growth of GaN nanowires, electrical resistance measurements (I-V), PL Imaging/Spectroscopy, microscopy (SEM), device fab via imprint lithography, analytical models of charge transport behavior, FE analysis.

- Hanchen Huang: MD, KMC, continuum mechanics (elasticity, plasticity), SEM, AFM imaging of physical systems (validation), visualization.

- Stephen Foiles: STM, HRTEM, MD, molecular statics, MC, LDA (DFT) VASP.

While this information can be organized and presented in a variety of ways, the list above demonstrates that presenters with expertise in either experimentation or modeling and simulation commanded an impressive knowledge of state-of-the-art techniques used by others outside of their expertise. In some instances, such as Ken Liechti, the presenter's knowledge of the strengths and limitations of both types of methods made it difficult to determine exactly where their expertise lies. Ken also demonstrated a mastery over the one tool that bridges experiments with modeling and simulation, that of communication. Ken's talk featured well over a dozen collaborators with expertise in both regimes, as well as a familiarity obtained through conversation and scientific literature. For other presenters, such as Stephen Foiles, while it was clear what methods the presenter mastered, it was equally clear that they had a familiarity and deep appreciation for knowledge gleaned through complementary methods. Again, this points to the use of communication as an effective research tool.

In addition to the ones listed above, participants also identified methods that they were familiar with but were not mentioned in the talks:

- Atomistic simulations methods for longer-time-scale events; infrequent events and jumps between metastable states
  - Hyperdynamics
  - Temperature accelerated dynamics
  - Parallel Replica dynamics
  - Free energy calculations
  - Stochastic MD
- 3D atom probe microscopy
- Dynamic diffractometer (10 ns resolution)
- Nanoindentation
- The broad spectrum of nanoscale characterization echniques that focus on nanoscale length, temporal, composition, and property resolution.

What are the major challenges of these methods that prevent the scientific community from doing predictive science?

This question was also easily answered by considering the comments made and questions asked during the technical presentations. While the list of challenges was monumental, further reflection shows they fall into four specific categories:

Improving the quality of interaction between experiment and modeling and simulation

More work is needed in establishing the validity of models and of modeling methods. This validation activity should not be a one-way road, but rather a feedback loop that connects modeling, experiment, and algorithm development. Experiments continue to provide the role of illuminating what phenomena are relevant to materials interfaces, and what aspects should be considered to gain a better understanding of these phenomena. Given that, theory and models should be used to guide experiments in a more consistent fashion. Too often, modelers use experimental work only for validation of their models and do not take an active enough role in deciding what aspects should be focused on with future experimental efforts. The question was also raised about how to incorporate algorithm development into this feedback loop. Historically, modelers and code developers have played the roles of ”customer” and ”supplier” with modelers communicating what needs their models have to the code development experts. It is unclear to what degree algorithm development requires input from models and simulations. Clearly, more advantage can be gained by using a feedback loop with regard to this interaction. At the least, those familiar with using implemented numerical tools can assist in situations where such tools may have direct benefit for experimentalists, and that line of communication exists in a limited way at best.

A point was also raised regarding serial versus parallel progression of research with multidisciplinary approaches. It was suggested that better planning of research efforts could produce multiple paths that minimize the ‘waiting time’ in using different approaches together.

During the discussion associated with this challenge, the question was also raised as to whether the terms ‘theorist’ and ‘modeler’ are synonymous? The definition of what ‘theoretical’ research constitutes seemed to vary among the different workshop participants. The subsequent conversation clarified that the term theorist is used to define those whose research focuses on conceptual and mathematical expressions and equations that describe physical phenomena. The solution of these equations can be obtained either analytically or through numerical approximations, and those whose research involves the latter activity are usually deemed 'modelers' (if they are responsible both for the derivation of the expressions/equations and for solving them) or 'analysts'.

Identifying and revising the boundaries of independence between experiment and modeling and simulation

Careful consideration should be applied in determining what the appropriate models and modeling methods should be for materials interface problems in which characterization unfeasible in experiments. In such instances, theoretical research should be designed along principles obtained by answering the questions: How can simulation be predictive without experiments? and Are there ways to improve the robustness of modeling methods without relying on experiment?

Equally important is that innovation be emphasized with regard to experimental capabilities. In particular, design of experiments is critical for materials issues for which modeling approaches are limited due to combinations of time-scale, length-scale and the ability to accurately the coupled physics and chemistry dominating the phenomena under examination. This does not preclude that improved capabilities in the modeling of multiple time scale processes are vitally needed and research should be encouraged.

Application of uncertainty quantification to multidisciplinary approaches

One challenge that became clear from the start of the workshop was that of perfecting both models and experimental techniques and obtaining statistics to establish their consistency. This concept of 'quantifying uncertainties' needs to be applied to both numerical models and experimental results. In particular, the workshop participants applauded efforts to characterize the statistics associated with material properties (whether measured in experiments or used as inputs for material models), but also put forward the immense challenge of applying statistical methods to methods that perform 'rigorous energy calculations. By doing this, we can better quantify the bounds of our predictive capabilities.

Adjacent to this challenge was the task of establishing the balance between the work associated with a computation, or an experiment, and its uncertainty. When a research path is considered, the balance of uncertainty versus accuracy must be performed in order to verify that the approaches used will yield the desired results.

Elements for constructing a predictive science capability

The final set of challenges identified all pertained to identifying what ingredients are essential towards building predictive science capabilities. Regarding the development of models, one issue to be solved is the identification of, and the development of solutions for, bottlenecks in multiscale approaches. For example, including accurate thermal conductivity behavior in atomistic systems, especially for metal systems, is still a vital capability, as are tools for overcoming the inherent time-scale limitation that exists for modeling of nanoscale phenomena. Also mentioned were new methods for 'downscale coupling', *i.e.* methods that can successfully transmit energy and information in large scale analyses to small scale simulations. This task is perhaps even more difficult than its opposite as methods to do this are not as ubiquitous in the scientific literature.

Also identified were issues related to implementation of models in simulation codes. In particular, more attention should be given to the development of efficient numerical algorithms and to deciding whether implementation within commercial codes or the construction of new task-specific codes was the better investment.

One challenge issued was that of building more rigorous connections between model development and the end application of materials design and predicting the outcome of materials processing. The concept of "simulation-based design" was repeatedly discussed and it was decided that while some success has been obtained with this approach (such as CRADA work that partnered Sandia with Goodyear), more work needs to be done to quantify the boundaries and qualify situation specific guidelines for future collaborations.

Finally, a missing element that makes experimentation as important to performing predictive science as modeling is the development and construction of new tools for manipulating nanoscale materials. Such tools will be critical, especially as the question of validation becomes increasingly relevant.

Can we identify the means to gauge the importance of the phenomena we study and the validity of the methods we use?

Several concrete suggestions were made towards answering this task:

- Perform iterative coupling of experiment and modeling & simulation. While this overlaps with some of the challenges listed in the previous question, it was made clear that confidence in research and approaches to research can be gained by using experiments and models to guide one another.

- Use dimensional analysis when analyzing your results.
- Attempt to define the bounds of uncertainty and validity when planning research, but also test these bounds as research proceeds.
- Use both 'bottom-up' and 'top-down' approaches to gauge importance when conducting research. Importance will be the convergence point of these different methodologies.
- Conduct parameter studies for both physical experiments and numerical simulations in order to accumulate statistics and estimate the sensitivity of phenomena to material properties and experiment/model attributes.
- Attempt to gain a better understanding of the underlying governing equations and principles.
- Pay attention to the larger scientific community, both in terms of what is being done (from scientific literature) and what is being funded (from agency communications and websites).

What are some new ways in which researchers with varied expertise, techniques and working environments can collaborate to stimulate innovative research?

The discussions conducted to answer this question were productive, and produced suggestions for actions to be taken at all levels of scientific and engineering research. For example, activities that can be initiated from the researcher level include using the web and internet resources to facilitate new collaborations, conducting and/or attending regular meetings and workshops on focused research areas, and participating in continuing education opportunities, especially with regard to education on techniques in disciplines outside of a researcher's area of expertise.

In concert with these efforts, it was also proposed that we need to communicate to higher levels the following:

- More funding opportunities are needed to initiate collaborations between academia, industry and national laboratories. This is not just a question of amount of money, but also pertains to where the money comes from. For example, it was pointed out that it may not be a coincidence that the nation's lack of high-tech leadership occurs during the same time in history for which there is a dwindling number of industry-directed research laboratories. There seems to be a limited phase space for funded collaborations that needs to be enlarged to stimulate innovative research. When proposing new opportunities, the funding architects should also contemplate the role of intellectual property (IP).

- Although innovation requires risk, the operational structure present in either academia or the laboratories may not be conducive to taking risk. New structures should be proposed and implemented. For example, rather than forming research groups around around traditional disciplinary fields, organization of groups by project, matrixing, co-location of theorists and experimentalists, etc., could be attempted.
- The workshop participants noticed the alarming trend of ever-decreasing time scale for newly funded research efforts. For current funding calls, the expectation of milestones and performance of reviews have compressed to the time scale of months. It is important that funding agencies and research directors realize that truly innovative research takes time, and an expanded time scale must be implemented to fertilize the creativity of scientific research. This could be accomplished through organized meetings with the purpose of educating those who control research funding and process, but who may not be researchers themselves, on the commitment necessary to perform and sustain high quality research.
- Continued activities like NECIS, with targeted programs to involve academia and lab staff, are essential to establishing new collaborations and innovative research environments. Elements of these programs include intern institutes, continuing education courses, opportunities for faculty work on-site at laboratory (2-week visits at a time), multi-participant projects, and variable timed visits (longer visits at initial stages, less frequent once collaboration becomes established). The activities can certainly be executed at the researcher level, as has been done with NECIS, but such programs **must** be supported at the highest levels in laboratories and research funding agencies.

How do we prepare both ourselves, and the next generation of scientists to do innovative research in interfaces?

The workshop participants brainstormed on this challenge and came up with the following ideas:

- Implement activities that involve both inter-disciplinary and multidisciplinary approaches to conducting research and education.

- Provide an appreciation for funding/management entities, thereby improving the scientific literacy of the research community.
- Using a different approach for basic science classes to make the material more accessible to the large community. This involves teaching a conceptual level of understanding of science and physical phenomena first before mathematical complexities are introduced. This approach reaches out to people at all levels of education and at all ages, even those without scientific or engineering background, thereby improving public support for research activities.
- Designing and implementing continuing education courses at institutions to help people get into new fields outside of their own disciplines. This can be done most effectively through programs such as CINT.
- Lower the barrier for industry researchers to attend external conferences and classes.
- Construct and maintain a repository of presentations, seminars, courses available online. This requires overcoming additional barriers on proprietary information for these courses in order to increase their availability.
- 'Speed dating' of researchers - Specialized social interactions that match researchers with various backgrounds and skill sets and attempt to maximize the number of collaborations that can be initiated.

Workshop Conclusions and Paths Forward

Conclusions

As the workshop came to a close Friday afternoon, the participants reflected on the expectations voiced during Wednesday night's discussion session and attempted to determine whether these expectations have been met:

- The desire for more information on how Sandia goes about conducting multidisciplinary research.

  It was made clear to the group that Sandia uses a combination of 'bottom-up' and 'top-down' approaches to create multidisciplinary collaborations. Sandians present mentioned that while the former approach was both commonly found and effective, more collaborations of the latter type are needed to direct research in the future. They also noted how colocation can be a huge asset with regard to making significant strides in multidisciplinary research.

- Whether inter-disciplinary training was advantageous with regard to training the next generation of scientists as compared with multidisciplinary partnerships?

  It was convincingly argued throughout the workshop that multidisciplinary partnerships of researchers trained extensively in specific fields and methods produced higher quality research than single individuals with inter-disciplinary training. However, cross-discipline courses were found to have a high value throughout a researcher's career.

- Is there a way to change the perspective of funding agencies and research calls from short-term projects to longer-term collaborations?

While this was certainly found to be an vital consideration, as discussed earlier in this report, it was not clear exactly how to accomplish this goal. That said, it is critical that the importance of this issue be communicated to higher level individuals, perhaps with the citing of specific, illustrative examples from previous decades of scientific and engineering research.

- How do we generate excitement and instill passion in our youth with regard to scientific and engineering research and development?

  Several suggestions were put forth with regard to this question, including:

  - Programs to do informal science education along with highlighted technology and innovation museums.
  - Increasing public relations for situations where the benefit of scientific research and technological innovation has benefited the average person. For example, the energy crises. This should especially be done for 'cool' applications of modern technology, *e.g.* surfboard foams. Another example is the use of quasi-scientific television programs to promote interest and enthusiasm. In particular, the CSI television series were mentioned as they've raised an awareness and an interest in forensic science among the general public. A similar media treatment in areas that intersect nanoscience and technology would be highly beneficial.
  - Initiating 'new' areas of research and new programs based on current events and infrastructure issues, *e.g.* the operation of the Alaska pipeline, technology for the war on terror.
  - Efforts are needed to provide the cultural impetus to have a career in engineering since the world environment has changed dramatically over the past two decades and the younger generation has easy access to information.
  - Summer camps and other outreach programs that generate knowledge and excitement on science and engineering.
  - Use the internet to present material at an accessible level for kids, *e.g.* MySpace.com.
  - Arrange two week visits to laboratories for middle and high school science teachers.
  - Programs by which laboratory staff visit schools and science classes.
  - Increased numbers and publicity for youth competitions such as math team competitions and science fairs.

– Develop and publicize a compelling and internationally competitive science and technology challenge. The most obvious example of this was the ”space race” back in the 1950's and 1960's in which American and Soviet resources were focused on getting vessels and people into space, and putting a man on the moon. This international competition had the indirect effect of motivating young people to pursue careers in science and engineering. A modern challenge is clearly needed to motivate the next generation.

Paths Forward

Participants also debated several options for paths forward on how to use what knowledge they'd obtained at the workshop and what conclusions their discussions led them to:

- Certainly, the workshop website should be maintained and the presentations and summary document should be added for public availability. In addition, the workshop organizing committee should be tasked with making sure the appropriate people are made aware of these materials.
- Sandia and those involved with the workshop plan to track collaborations, project proposals, etc, over a 6 mos - 1 year span. This will help provide evidence as to the long-term effectiveness of the workshop.
- E-mail communication and internet methods will be used to facilitate action plans for some efforts suggested, *e.g.* internet reach-out, summer camps, etc.
- All workshop participants should shoulder some responsibility in communicating (verbally and through documentation) concerns about funding, research time-lines, etc to funding agencies/officials, management, and university leaders.
- Efforts should be maintained and increased to support and run programs that facilitate academic-lab collaboration, especially with faculty and staff and for multi-participant collaborations.
- Future workshops should be conducted that more targeted on specific technical problems.

The final question raised during the workshop was “Is nanoscience sufficient to generate excitement at the national level?” This group of scientists, engineers, and managers believes so, but specific ties to technology must be pointed out. Also, as a community we should encourage those that embrace the imaginative potential of nanotechnology and use this imagination to support motivation in this important research area.